IR divergence does not affect the gauge-invariant curvature perturbation

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We address the infrared(IR) divergence problem during inflation that appears in the loop corrections to the primordial perturbations. In our previous paper, we claimed that, at least in single field models, the IR divergence is originating from the gauge artifact. Namely, diverging IR corrections should not appear in genuine gauge-invariant observables. We propose here one simple but explicit example of such gauge-invariant quantities. Then, we explicitly calculate such a quantity to find that the IR divergence is absent at the leading order in the slow-roll approximation for the usual scale invariant vacuum state. At the same time we notice that there is a subtle issue on the gauge-invariance in how to specify the initial vacuum state.

I. INTRODUCTION

The precise measurements of the primordial fluctuation provide us with valuable information of the early universe. It is widely accepted that the primordial fluctuation originates from the quantum fluctuation of the inflaton field. In the last decades, it has been recognized that the perturbation theory in the inflationary universe might break down because of the infrared(IR) divergence from loop corrections [1]. (For a recent review, see Ref. [2].) During inflation, massless fields are known to yield the scale invariant spectrum $P(k) \propto 1/k^3$ at linear order. These fields contribute to the one-loop diagram with the four point interaction as $\int \mathrm{d}^3k/k^3$, which leads to the logarithmic divergence.

It has been an issue of debate whether the IR divergences are physical or not. If it were really physical, there might be a possibility that loop corrections are observable. The possibility of secular growth of IR contributions has also been studied motivated as a possible explanation of the smallness of the cosmological constant [3]. However, before we discuss implications of the IR effects, we need to carefully examine whether the reported IR divergences are not due to careless treatment. (See also Ref. [4])

In our previous work [5], we pointed out the presence of gauge degrees of freedom in the frequently used gauges such as the comoving gauge and the flat gauge, and these gauge degrees of freedom are responsible for the IR divergences. There, we have shown that, if we fix the residual gauge degrees of freedom, the IR divergences automatically disappear in the single field model. (Multi-field case was discussed in a separate paper [6].)

In this paper, we reexamine our previous argument. If the IR divergences are really due to the residual gauge degrees of freedom, those divergences should disappear if we evaluate genuine gauge-invariant quantities even though we do not fix the residual gauge. Hence, the demonstration of the genuine gauge-invariance of computed results would be necessary to obtain reliable predictions, which are to be compared with observations. In this brief report we demonstrate more explicitly that the IR divergence in the curvature perturbation can be removed by looking at such genuine gauge-invariant quantities. In doing so, we shall notice that the choice of initial vacuum state is restricted. In the slow roll limit, we find that a natural

vacuum state is surprisingly limited to the Bunch-Davies vacuum state as far as we consider Gaussian vacuum state for the inflaton perturbation in the flat slicing at the initial time.

II. BASIC EQUATIONS

We consider the single field inflation model whose action takes the form

$$S = \frac{M_{\rm pl}^2}{2} \int \sqrt{-g} \left[R - g^{\mu\nu} \phi_{,\mu} \phi_{,\nu} - 2V(\phi) \right] d^4 x , \quad (1)$$

where $M_{\rm pl}$ is the Planck mass and the scalar field Φ was rescaled so as to be non-dimensional as in Ref. [5]. Substituting the metric form

$$ds^{2} = -N^{2}dt^{2} + h_{ij}(dx^{i} + N^{i}dt)(dx^{j} + N^{j}dt), \quad (2)$$

the action becomes

$$S = \frac{M_{\rm pl}^2}{2} \int \sqrt{h} \left[N^s R - 2NV(\phi) + \frac{1}{N} (E_{ij} E^{ij} - E^2) + \frac{1}{N} (\dot{\phi} - N^i \partial_i \phi)^2 - N h^{ij} \partial_i \phi \partial_j \phi \right] d^4 x , (3)$$

where E_{ij} and E are defined by

$$E_{ij} = \frac{1}{2} \left(\dot{h}_{ij} - D_i N_j - D_j N_i \right), \quad E = h^{ij} E_{ij} .$$
 (4)

In this paper we work in the comoving gauge, defined by $\delta\phi=0$. We decompose the spatial metric as

$$h_{ij} = e^{2(\rho+\zeta)}\gamma_{ij} = e^{2(\rho+\zeta)} \left[e^{\delta\gamma}\right]_{ij} , \qquad (5)$$

where $a:=e^{\rho}$ is the background scale factor, and $\mathrm{tr}[\delta\gamma]=1$. Using the degrees of freedom of choosing the spatial coordinates, we further impose the gauge conditions $\partial^i \delta \gamma_{ij}=0$.

Varying the action with respect to N and N^i , we obtain the Hamiltonian and momentum constraints as

$${}^{s}R - 2V - N^{-2}(E^{ij}E_{ij} - E^{2}) - N^{-2}\dot{\phi}^{2} = 0$$
, (6)

$$D_{j} \left[N^{-1} \left(E^{j}{}_{i} - \delta^{j}{}_{i} E \right) \right] = 0.$$
 (7)

For convenience, we factorize the scale factor from the metric

$$ds^{2} = e^{2\rho} \left[-(N^{2} - \check{N}_{i}\check{N}^{i})d\eta^{2} + 2\check{N}_{i}d\eta dx^{i} + \check{h}_{ij}dx^{i}dx^{j} \right],$$

where we have defined $\check{h}_{ij}:=e^{-2\rho}h_{ij}=e^{2\zeta}\gamma_{ij}, \ N_i=e^{\rho}\check{N}_i,$ and $\check{N}^i:=\check{h}^{ij}\check{N}_i=e^{\rho}N^i.$ Expanding the perturbations, $\mathfrak{Q}=\delta N(:=N-1), \check{N}_i, \zeta,$ and $\delta\gamma_{ij}$ as $\mathfrak{Q}=\mathfrak{Q}_1+\frac{1}{2}\mathfrak{Q}_2+\cdots$, the zeroth-order Hamiltonian constraint equation yields the background Friedmann equation:

$$6\rho'^{2} = \phi'^{2} + 2\check{V}(\phi), \qquad (8)$$

where a prime "'" denotes the differentiation with respect to the conformal time η , and $\check{V}(\phi) := e^{2\rho}V(\phi)$. The constraint equations at the linear order are obtained as

$$\check{V}\delta N_1 - 3\rho'\zeta_1' + \partial^2\zeta_1 + \rho'\partial^i \check{N}_{i,1} = 0, \qquad (9)$$

$$4\partial_i \left(\rho' \delta N_1 - \zeta_1' \right) - \partial^2 \check{N}_{i,1} + \partial_i \partial^j \check{N}_{j,1} = 0. \quad (10)$$

The higher-order constraints can be obtained similarly.

III. ORIGIN OF IR DIVERGENCE

A. Influence of boundary conditions

Solving the constraints (6) and (7), we can express δN and N_i in terms of the curvature perturbation ζ . Here we stress that the constraints (9) and (10) are elliptic-type equations, which require boundary conditions to solve. Below we study the relation between the residual gauge degrees of freedom and the integration constants appearing in the general solution of Eqs. (6) and (7). For illustrative purpose, we consider the linear order, in which constraints are given by Eqs. (9) and (10), but the extension to higher orders proceeds in a similar manner

Eliminating δN_1 from Eqs. (9) and (10), we obtain

$$\left(1 - \frac{4\rho'^{2}}{\check{V}}\right) \partial_{i}\partial^{j}\check{N}_{j,1} - \partial^{2}\check{N}_{i,1} + 2\frac{\phi'^{2}}{\check{V}}\partial_{i}\zeta_{1}' - 4\frac{\rho'}{\check{V}}\partial_{i}\partial^{2}\zeta_{1} = 0.$$
(11)

Taking the divergence of Eq. (11), the longitudinal part of $N_{i,1}$ is solved as

$$\partial^{i} \check{N}_{i,1}(x) = \frac{\phi'^{2}}{2\rho'^{2}} \zeta'_{1}(x) - \frac{1}{\rho'} \partial^{2} \zeta_{1}(x) + F_{1}(x) , \quad (12)$$

where $F_1(x)$ is an arbitrary solution of the Laplace equation. Using Eqs. (11) and (12), $N_{i,1}$ is integrated to give

$$\tilde{N}_{i,1}(x) = \partial_i \left(\frac{{\phi'}^2}{2{\rho'}^2} \partial^{-2} \zeta_1'(x) - \frac{1}{{\rho'}} \zeta_1(x) \right) \\
+ \left(1 - \frac{4{\rho'}^2}{\check{V}} \right) \partial_i \partial^{-2} F_1(x) + G_i(x) , (13)$$

where $G_i(x)$ is an arbitrary vector that satisfies $\partial^2 G_i(x) = 0$. Here we assumed that the inverse Laplacian ∂^{-2} is defined uniquely. Comparing the divergence of Eq. (13) with Eq. (12), we find $F_1(x) = (\tilde{V}/4\rho'^2)\partial^i G_i(x)$. Substituting Eq. (12) into Eq. (10), the lapse function is easily obtained. To conclude, the lapse function and the shift vector are given by

$$\delta N_{1} = \frac{1}{\rho'} \left(\zeta_{1}' - \frac{1}{4} \partial^{i} G_{i} \right) , \qquad (14)$$

$$\tilde{N}_{i,1} = \partial_{i} \left(\frac{{\phi'}^{2}}{2{\rho'}^{2}} \partial^{-2} \zeta_{1}' - \frac{1}{\rho'} \zeta_{1} \right)$$

$$- \frac{1}{4} \left(1 + \frac{{\phi'}^{2}}{2{\rho'}^{2}} \right) \partial_{i} \partial^{-2} \partial^{j} G_{j} + G_{i} . \qquad (15)$$

Introduction of a vector $G_i(x)$ also modifies the evolution equations of the curvature perturbation ζ and the transverse-traceless perturbation $\delta \gamma_{ij}$. Substituting Eqs. (14) and (15) into Einstein equations, we obtain

$$(\zeta_1 - f_1)'' + 2(\ln z)'(\zeta_1 - f_1)' - \partial^2(\zeta_1 - f_1) = 0$$
, (16)

where we have defined $z:=e^{\rho}\phi'/\rho'$ and $f_1(x):=\frac{1}{4}\int \mathrm{d}\eta\,\partial^i G_i(x)$, which implies $\partial^2 f_1(x)=0$. While the evolution equation of $\delta\gamma_{ij}$ is obtained as

$$\delta\gamma_{ij,1}'' + 2\rho'\delta\gamma_{ij,1}' - \partial^2\delta\gamma_{ij,1}$$

$$-\left(\frac{\phi'}{\rho'}\right)^2\partial_i\partial_j(\partial^{-2}\partial^2 - 1)\zeta_1 + \frac{1}{2\rho'}\partial_i\partial_j\partial^kG_k$$

$$-e^{-2\rho}\partial_\eta\left\{e^{2\rho}(\partial_iG_j + \partial_jG_i - \frac{1}{2}\partial_i\partial_j\partial^{-2}\partial^kG_k - \frac{1}{2}\partial^kG_k\delta_{ij})\right\} = 0. (17)$$

This equation is consistent with the transverse traceless condition of $\delta\gamma_{ij}$. Namely, the trace and divergence of Eq. (17) are automatically satisfied. These evolution equations of ζ_1 and $\delta\gamma_{ij,1}$ reduce to the ordinary well-known linear perturbation equations by simply setting $G_i=0$.

When we consider the universe with infinite volume, the solution of δN_1 and $\check{N}_{i,1}$ would be specified uniquely by the requirement that all quantities are regular at the spatial infinity. In this case, we have not room to introduce $G_i(x)$. In contrast, when we concentrate on a finite region of the universe, a variety of solutions are allowed especially due to the presence of homogeneous solutions of Laplace equation. In this case, as presented by the first term in the second line of Eq. (17), it also happens that the evolution equation for the transverse traceless mode $\delta\gamma_{ij}$ is contaminated by the longitudinal mode ζ , even at the linear order.

B. Gauge degrees of freedom

The ambiguity in the choice of the vector G_i indicates the presence of residual gauge degrees of freedom. Here, we show explicitly that $G_i(x)$ represents the residual gauge degrees of freedom that remain even after we specify the gauge by $\delta \phi = 0$ and the conditions (5). Since the condition $\delta \phi = 0$ completely fixes the temporal gauge, we are only allowed to

change the spatial coordinates. Under the change of the spatial coordinates $x^i \to x^i + \delta x^i$, the metric functions transform as

$$\tilde{\tilde{N}}_{i,1}(x) = \tilde{N}_{i,1}(x) - \delta x_i' \,, \tag{18}$$

$$\tilde{\zeta}_1(x) = \zeta_1(x) - \frac{1}{3}\partial^i \delta x_i , \qquad (19)$$

$$\delta \tilde{\gamma}_{ij,1} = \delta \gamma_{ij,1} - \left(\partial_i \delta x_j + \partial_j \delta x_i - \frac{2}{3} \partial^k \delta x_k \delta_{ij} \right) ,$$
 (20)

where $\delta x_i := \delta_{ij} \delta x^j$. We associate a tilde with the perturbed variables when we set $G_i \neq 0$ to discriminate them from those in the gauge with $G_i = 0$. Recalling that the lapse function remains unchanged, the comparison between Eqs. (14) and (19) gives

$$\partial^i \delta x_i' = -(3/4)\partial^i G_i(x) . (21)$$

Imposing the transverse condition of $\delta \gamma_{ij}$ in Eq. (20) yield

$$\partial^2 \delta x_i = -(1/3)\partial_i \partial^j \delta x_i . ag{22}$$

Comparing Eq. (15) with Eq. (18) together with Eqs. (21) and (22), δx_i is solved as (See Ref. [7].)

$$\delta x_{i}(x) = -\int d\eta G_{i}(x) + \frac{1}{4} \int d\eta \partial_{i} \partial^{-2} \partial^{j} G_{j}(x)$$

$$+ \frac{1}{4} \int \frac{d\eta}{\rho'} \int d\eta \partial_{i} \partial^{j} G_{j}(x) + H_{i}(x)$$

$$+ \int \frac{d\eta}{\rho'} \partial^{2} H_{i}(x) , \qquad (23)$$

where we introduced a vector $H_i(x)$ that satisfies

$$3\partial^2 H_i(\mathbf{x}) + \partial_i \partial^j H_i(\mathbf{x}) = 0.$$
 (24)

Substituting Eq. (23) into Eqs. (19) and (20), we find that spatial components of metric perturbation transform as

$$\tilde{\zeta}_{1} = \zeta_{1} + \frac{1}{4} \int d\eta \, \partial^{i} G_{i} - \frac{1}{3} \partial^{i} H_{i} .$$

$$\delta \tilde{\gamma}_{ij,1} = \delta \gamma_{ij,1} + \int d\eta \left\{ 2 \partial_{(i} G_{j)} - \frac{1}{2} (\partial_{i} \partial_{j} \partial^{-2} + \delta_{ij}) \partial^{k} G_{k} \right\}$$

$$- \frac{1}{2} \int \frac{d\eta}{\rho'} \int d\eta \partial_{i} \partial_{j} \partial^{k} G_{k} - 2 \left(\partial_{(i} H_{j)} - \frac{1}{3} \partial^{k} H_{k} \delta_{ij} \right)$$

$$- 2 \int \frac{d\eta}{\rho'} \partial^{2} \partial_{(i} H_{j)} .$$
(25)

To remedy the IR divergence due to the gauge modes, in our previous work [5, 6], we proposed to use the local gauge condition such that the effects from the causally disconnected region are shut off. The local gauge condition can be achieved by choosing the function $G_i(x)$ appropriately. To remove the IR divergence explicitly, the residual gauge must be fixed so that $\tilde{\zeta}$ measures the deviation from the average value taken over a certain local region $\mathbb O$. In Ref. [5], we have shown that the IR corrections become finite by adopting this local gauge. In this gauge IR contributions are effectively cut off at the length scale of the size of $\mathbb O$. However, one can change the choice of $\mathbb O$, which leads to a finite shift in the gauge function $G_i(x)$. As a result, the resulting correlation functions for $\tilde{\zeta}$

depend on the artificial choice of O. This prescription will be sufficient just to show that the loop corrections are finite in some gauge, but it will not be sufficient to evaluate the size of loop corrections. In the present work, we give an example of genuine gauge-invariant quantities that do not depend on how we fix the residual gauge degrees of freedom. The expected correlations in the CMB temperature fluctuations should be also such gauge-invariant quantities.

IV. GAUGE INVARIANCE AND IR REGULARITY

A. Construction of gauge-invariant variables

In this subsection, we construct an example of genuine gauge-invariant quantities. Since the temporal slicing is already fixed, it is sufficient to address the gauge-invariance under the residual gauge transformation of the spatial coordinates (23). Genuine gauge-invariance is equivalent to complete gauge fixing. In this sense, if we give appropriate boundary conditions for the lapse and shift, the residual gauge degrees of freedom can be completely fixed. However, here arises a difficulty in fixing the gauge, because we need to remove all arbitrariness regarding the choice of coordinates, such as the choice of the local region O.

When we consider the universe with infinite volume, the conventional gauge-invariant perturbation theory is formulated using particular combinations of perturbed variables invariant under an arbitrary gauge transformation. The construction of such gauge-invariant variables is possible thanks to the absence of the ambiguity in the inverse Laplacian under the assumption that the perturbations remain finite at the spatial infinity. However, the same procedure does not work when we try to use only the information contained in the limited area \odot . Under this restriction, genuine gauge-invariant quantities cannot be constructed by the combination of local quantities.

Keeping these in mind, we consider n-point functions of the scalar curvature sR . The scalar curvature sR does not remain invariant but transforms as a scalar quantity under the change of spatial coordinates. If we could specify its n arguments in a coordinate-independent manner, the n-point functions of sR would be gauge-invariant. This can be partly achieved by specifying the n spatial points by the geodesic distances and the directional cosines from one reference point. Although we cannot specify the reference point in a coordinate independent manner, this gauge dependence would not matter as long as we are interested in the correlation functions for a quantum state that respects the spatial homogeneity and isotropy of the universe.

As an example, we consider the two point function of sR , whose arguments X_A^i (A=1,2) are specified by solving the three-dimensional geodesic equation from $\lambda=0$ to 1 with the initial "velocity" $\mathrm{d} X_A^i(\lambda)/\mathrm{d} \lambda|_{\lambda=0}=x_A^i$ starting with the origin. We denote $X_A^i(\lambda=1)$ simply by X_A^i , which can be perturbatively expanded as $X_A^i:=x_A^i+\delta x_A^i$. x_A^i can be understood as the background value of the points. Then, the

expectation value of a product of

$${}^{g}R(\eta, x_A^i) := {}^{s}R(\eta, x_A^i + \delta x_A^i)$$

$$= \sum_{n=0}^{\infty} \frac{\delta x_A^{i_1} \cdots \delta x_A^{i_n}}{n!} \partial_{i_1} \cdots \partial_{i_n} {}^{s}R(\eta, x_A^i), (27)$$

should be gauge-invariant.

B. IR regularity of genuine gauge-invariants

The genuine gauge-invariant quantities we introduced should be finite in the local gauge, since the field itself is constructed to be free from IR divergence in this gauge by construction. However, since these quantities are really gauge-invariant, they should be finite even if we send the size of $\mathbb O$ to infinity. This limit is supposed to agree with the case when we calculate them in the infinite volume [7]. In the rest of this paper we study the regularity of the gauge-invariant two point function introduced above in the conventional global gauge [8], focusing on the loop of longitudinal modes at the lowest order in the slow-roll approximation. The spatial curvature sR is given by

$${}^{s}R = -2e^{-2(\rho+\zeta)}(2\partial^{2}\zeta + \partial_{i}\zeta\partial^{i}\zeta). \tag{28}$$

We expand the gauge-invariant spatial curvature as ${}^gR = {}^gR_1 + {}^gR_2 + \cdots$, in terms of the interaction picture field operator. Here the subscript denotes the number of the operators. Then, one-loop contribution to the two point function starts with the quartic order,

$$\langle {}^{g}R^{g}R\rangle_{4} := \langle {}^{g}R_{1}{}^{g}R_{3}\rangle + \langle {}^{g}R_{2}{}^{g}R_{2}\rangle + \langle {}^{g}R_{3}{}^{g}R_{1}\rangle. \tag{29}$$

Using the fact that the IR divergence arises only from the contraction between interaction picture fields without any derivative, we keep only the terms that are possibly divergent. For instance, the terms that include more than two interaction picture fields with spatial or temporal derivatives do not yield divergences.

In order to obtain the expression for ${}^s\!R$, we use the fact that in the flat slicing the interaction Hamiltonian is totally suppressed by the slow roll parameter [8]. We therefore solve the non-linear evolution of perturbation in the flat gauge, and transform the results into the $\delta\phi=0$ gauge. Then, the contributions at the lowest order in slow-roll expansion to ζ arises only from the non-trivial gauge transformation given by [8]

$$\zeta = \zeta_n + \frac{1}{2\rho'}\zeta_n'\zeta_n + \frac{1}{2{\rho'}^2}\zeta_n''\zeta_n^2 + \cdots,$$
 (30)

where $\zeta_n := -\rho' \varphi_I/\phi'$ and the abbreviated terms are higher order or irrelevant for the divergences. Here φ_I is the interaction picture field corresponding to the inflaton perturbation in the flat gauge.

Solving the spatial geodesic equation on a $\eta=$ constant hypersurface, we obtain $X^i=e^{-\zeta}x^i+\cdots$, where the terms with spatial differentiations were abbreviated since they do not contribute to the possible IR divergence in $\langle {}^gR^gR \rangle_4$. After

some manipulations, the possibly divergent terms in $\langle {}^g\!R^g\!R \rangle_4$ can be summed up as

$$\langle {}^{g}R(x){}^{g}R(y)\rangle_{4} \propto \langle \zeta_{n}^{2}\rangle \int \mathrm{d}(\log k) \left[D^{2}u_{\mathbf{k}}(x)u_{\mathbf{k}}^{*}(y) + 2Du_{\mathbf{k}}(x)Du_{\mathbf{k}}^{*}(y) + u_{\mathbf{k}}(x)D^{2}u_{\mathbf{k}}^{*}(y)\right] + (\mathbf{c.c.}). \tag{31}$$

where $u_{\boldsymbol{k}}(x)$ is the positive frequency function of the field ζ_n multiplied by $k^{7/2}$, and D is an operator defined by $D:=\eta\partial_\eta+x^i\partial_i+2$. Since $\langle\zeta_n^2\rangle$ is IR divergent, the regularity is maintained only when the integral in (31) vanishes exactly. If we use the scale-invariant property of mode functions of the Bunch-Davies vacuum, the derivative operator D acting on $u_{\boldsymbol{k}}$ is replaced with $\partial_{\log k}$. Then, this integral becomes total derivative and vanishes. The usage of the invariant distance is requested also in Ref. [9], where the δN formalism is utilized. It is intriguing that, while the method is different, they have arrived at the same conclusion as we have.

One may think it strange to require the scale-invariance, because genuine gauge-invariant correlation functions should be finite independent of the choice of initial vacuum state. This finiteness is guaranteed as long as we compute it in the local gauge. This gauge dependence stems from that of the initial vacuum state. In Ref. [5] we implicitly specified the initial vacuum state so that the interaction picture field is identical to the Heisenberg field on the initial surface. Namely, the interaction is assumed to be turned off before the initial time. Since the effect of the coordinate transformation on the perturbation variables is non-linear, this identification between the Heisenberg field and the interaction picture field has different meaning depending on the choice of gauge. Therefore, in order to obtain genuine gauge-invariant results, we need the principle to specify the vacuum state in a gauge-invariant manner. If we specify the initial state so that the interaction picture field is identical to the Heisenberg field at the initial time in the local gauge, the selected quantum state depends on the choice of the local volume O. This situation is unsatisfactory. Moreover, such a choice of vacuum will violate the three-dimensional translational invariance. Hence, it is much favoured to specify the initial vacuum state in the global gauge. As we have seen above, at the lowest order of slow roll approximation, the scale-invariant Bunch-Davies vacuum state is such a vacuum state that is free from IR divergences. Since the origin of the possible IR divergence is confined to the initial vacuum state, we may say that, if genuine gauge-invariant correlation functions of fluctuations are free from divergence at the initial time, it remains so in the course of time evolution. However, the extension of a natural vacuum free from IR divergence to the higher order in slow-roll expansion does not seem trivial at all. In this brief report we have also neglected the transversetraceless metric perturbation, which can participate in the IR divergence. These issues will be discussed in our future publication [7].

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